

IN THE CLAIMS:

This listing of claims replaces all prior versions and listings of claims in the application:

Listing of Claims

Claims 1-8. (Canceled)

9. (Currently Amended) A computer-assisted method for determining a three-dimensional structure of a target protein using a computer comprising a processor configured to receive and output data in accordance with executable code, the method comprising:

- (a) generating input data for the computer comprising:
 - (i) inputting as a string of an identity constraint and a secondary structure constraint and/or tertiary constraints for some or all of the amino acid residues ~~residue~~ comprising the target protein; and
 - (ii) by way of executable code, directing the processor to produce from the string a three dimensional reduced protein model comprised of representations of side chains of the amino acid residues comprising the target protein wherein said representations of side chains of amino acid residues are converted to interaction centers and each interaction center comprises a pseudoatom representing a center of mass of the side chain of the represented amino acid to which the interaction center corresponds, and each interaction center is connected to an immediately proximal interaction center and an immediately distal interaction center via a virtual covalent bond to produce an interaction center chain, which is projected onto an underlying cubic lattice to produce a projected chain of interaction centers, and then secondary constraints and/or tertiary constraints are applied to a subset of, or all of, the interaction centers of the interaction center chain to generate a knowledge based origin comprising a force field of short-

range interactions, thereby producing a data set representing a three-dimensional model structure of the target protein; and

(b) outputting the three dimensional reduced protein model to an output device or a storage device.

10. (Original) A method according to claim 9 wherein the secondary structure constraint for each amino acid residue is selected from the group of "H" for helix, "E" for extended, and "(i)" for other structural constraints.

11. (Original) A method according to claim 9 wherein the secondary structural constraint for a subset of amino acid residues comprising the target protein is generated by a threading alignment of an amino acid sequence of the target protein.

Claims 12-13. (Canceled)